1-1-2006

Mathematical modelling for a C60 carbon nanotube oscillator

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Abstract

The discovery of fullerenes C_{60} and carbon nanotubes has created an enormous impact on nanotechnology. Because of their unique mechanical and electronic properties, such as low weight, high strength, flexibility and thermal stability, fullerenes C_{60} and carbon nanotubes are of considerable interest to researchers from many scientific areas. One problem that has attracted much attention is the creation of gigahertz oscillators. While there are difficulties for micromechanical oscillators, or resonators, to reach a frequency in the gigahertz range, it is possible for nanomechanical systems to achieve this. A number of studies have found that the sliding of the inner-shell inside the outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies up to several gigahertz. In addition, it has been observed that the shorter the inner tube, the higher the frequency, leading to the introduction of a C_{60}-nanotube oscillator. Thus instead of multi-walled carbon nanotubes, high frequencies can be generated using a fullerene C_{60} oscillating inside a single-walled carbon nanotube. In this paper, using the Lennard-Jones potential, we determine the potential for an offset C_{60} molecule inside a single-walled carbon nanotube, so as to determine its position with reference to the cross-section of the carbon nanotube. The condition for the C_{60} initially at rest outside the carbon nanotube to be sucked in and to start oscillating is also presented together with a mathematical model for the resulting oscillatory motion. This paper summarizes recent results obtained by the present authors.

Keywords

Mathematical, modelling, for, C60, carbon, nanotube, oscillator

Disciplines

Physical Sciences and Mathematics

Publication Details

Cox, B. J., Thamwattana, N. & Hill, J. M. (2006). Mathematical modelling for a C60 carbon nanotube oscillator. In C. Jagadish & G. Lu (Eds.), Proceedings of 2006 International Conference On Nanoscience and Nanotechnology (pp. 80-83). USA: IEEE.

Mathematical Modelling for a C_{60} Carbon Nanotube Oscillator

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***Abstract*—The discovery of fullerenes C_{60} and carbon nanotubes has created an enormous impact on nanotechnology. Because of their unique mechanical and electronic properties, such as low weight, high strength, flexibility and thermal stability, fullerenes C_{60} and carbon nanotubes are of considerable interest to researchers from many scientific areas. One problem that has attracted much attention is the creation of gigahertz oscillators. While there are difficulties for micromechanical oscillators, or resonators, to reach a frequency in the gigahertz range, it is possible for nanomechanical systems to achieve this. A number of studies have found that the sliding of the inner-shell inside the outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies up to several gigahertz. In addition, it has been observed that the shorter the inner tube, the higher the frequency, leading to the introduction of a C_{60}-nanotube oscillator. Thus instead of multi-walled carbon nanotubes, high frequencies can be generated using a fullerene C_{60} oscillating inside a single-walled carbon nanotube. In this paper, using the Lennard-Jones potential, we determine the potential for an offset C_{60} molecule inside a single-walled carbon nanotube, so as to determine its position with reference to the cross-section of the carbon nanotube. The condition for the C_{60} initially at rest outside the carbon nanotube to be sucked in and to start oscillating is also presented together with a mathematical model for the resulting oscillatory motion. This paper summarizes recent results obtained by the present authors.**

Keywords-carbon nanotubes; fullerenes C_{60}; gigahertz oscillators; Lennard-Jones potential

I. INTRODUCTION

Carbon nanotubes have many promising applications in new technological devices including in optical, mechanical and electrical systems. This is due to their size and their unique properties, such as high strength, low weight, flexibility and thermal stability. Recently, it has been found that the oscillating of the inner tube of a multi-walled carbon nanotube can generate the oscillatory frequencies in the gigahertz range. This finding leads to many potential applications, such as ultra-fast optical filters and nano-antennae.

Cumings and Zettl [1] experiment on multi-walled carbon nanotubes, where they remove the cap from one end of the outer-shell and attach a moveable nanomanipulator to the core in a high-resolution transmission electron microscope (TEM). By pulling the core out and pushing it back into the outer-shell, they report an ultra low frictional force against the intershell sliding. This result is also confirmed by Yu, Yakobson and Ruoff [2]. Further, Cumings and Zettl [1] also observe that the extruded core, after release, quickly and fully retracts inside the outer-shell due to the restoring force resulted from the van der Waals interaction acting on the extruded core. These results led Zheng and Jiang [3] and Zheng, Liu and Jiang [4] to study the molecular gigahertz oscillators, where the sliding of the inner-shell inside the outer-shell of a multi-walled carbon nanotube can generate oscillatory frequencies up to several gigahertz.

Based on Zheng et al. [4], which state that the shorter the inner tube, the higher the frequency, instead of using the inner tube Liu, Zhang and Lu [5] find that the high frequency can be generated by the oscillating of a fullerene C_{60} inside a single-walled carbon nanotube. A fullerene C_{60} is a stable carbon structure, where sixty carbon atoms bond to form an approximate sphere. For further details of fullerenes, we refer the reader to Dresselhaus, Dresselhaus and Eklund [6]. While Liu et al. [5] and Qian, Liu and Ruoff [7] study a C_{60}-nanotube oscillator using molecular dynamical simulations, Cox, Thamwattana and Hill [8, 9] employ elementary mechanics and mathematical modelling techniques to investigate this problem and this is the main contribution of the authors in the area. Further, the results obtained in Cox et al. [8, 9] are in a good agreement with numerical results of Girifalo, Hodak and Lee [10] and Hodak and Girifalco [11], and molecular dynamical simulations of Liu et al. [5] and Qian et al. [7]. Here, we review Cox et al. [8, 9], and summarize the essential mechanisms of a C_{60}-nanotube oscillator. For full details of the mathematical derivations, we refer the reader to Cox et al. [8, 9].

II. POTENTIAL FUNCTION

In the continuum approximation, carbon atoms are assumed to be uniformly distributed over the surface of the molecules. As a result, the nonbonded interaction energy between two molecules is obtained by integrating the interaction energy $\Phi(r)$ over the surfaces of each entity, namely

$$E = n_g n_f \iint \Phi(r) d\Sigma_g d\Sigma_f, \tag{1}$$

where n_g and n_f denote the mean surface density of atoms on a carbon nanotube and a fullerene C_{60}, respectively, and r is the distance between two typical surface elements $d\Sigma_g$ and $d\Sigma_f$ on each molecule. In this paper, we adopt the well-known Lennard-Jones potential

$$\Phi(r) = -Ar^{-6} + Br^{-12}, \tag{2}$$

where A and B denote the attractive and repulsive constants respectively. Here, we use A = 17.4 eVÅ^6 and B = 29×10^3 eVÅ^{12} for the interaction between C_{60}-graphene (Girifalco et al. [10]).

III. Interaction of a C_{60} Fullerene Located on the Axis of a Single-walled Carbon Nanotube

By using (1) and (2), we find the potential of an atom on the carbon nanotube of radius a interacting with all atoms of the spherical fullerene of radius b to be given by

$$P(\rho) = n_f \pi b A\left[(\rho+b)^{-4} - (\rho-b)^{-4}\right]\Big/(2\rho) - n_f \pi b B\left[(\rho+b)^{-10} - (\rho-b)^{-10}\right]\Big/(5\rho), \quad (3)$$

where ρ is the distance between the centre of the C_{60} molecule and an atom on the carbon nanotube, as shown in Fig. 1.

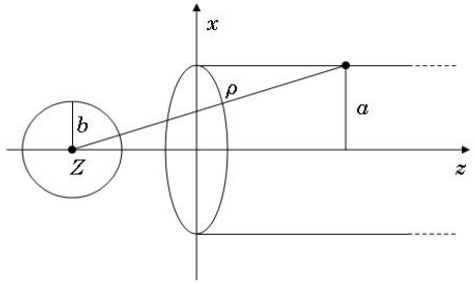

Figure 1. Geometry of a fullerene entering a carbon nanotube

The van der Waals interaction force between the fullerene molecule and an atom on the tube is given by $F_{vdW} = -\nabla P$, thus from Fig. 1 the axial force is of the form

$$F_z = -\frac{(Z-z)}{\rho}\frac{dP}{d\rho}. \quad (4)$$

As a result, the total axial force $F_z^{tot}(Z)$ of the entire carbon nanotube ($0 \le z < \infty$) interacting with the fullerene can be obtained by performing surface integral of (4) over the tube, which upon simplifying, we have

$$F_z^{tot}(Z) = \frac{8\pi^2 n_f n_g a}{b^4\lambda^3}\left[A\left(1+\frac{2}{\lambda}\right) - \frac{B}{5b^6\lambda^3}\left(5+\frac{80}{\lambda}+\frac{336}{\lambda^2}+\frac{512}{\lambda^3}+\frac{256}{\lambda^4}\right)\right], \quad (5)$$

where $\lambda = (a^2 - b^2 + Z^2)/b^2$. In Fig. 2, we plot (5) and find that equation $F_z^{tot}(Z) = 0$ admits at most two real roots, $Z = \pm Z_0$, when the radius a is less than some critical value a_0, where b is given. In the case of a C_{60} fullerene (b = 3.55 Å) then a_0 = 6.509 Å. We note from the form of (5) that Z only appears in factors of Z^2. Therefore, the force is symmetrical about $Z = 0$.

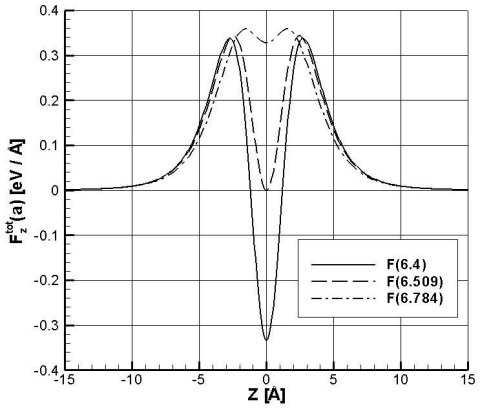

Figure 2. Force experienced by a C_{60} molecule due to van der Waals interaction with a semi-infinite carbon nanotube

The integral of $F_z^{tot}(Z)$ represents the work imparted to the fullerene and equates directly to the kinetic energy. Therefore, integral of F_z^{tot} from $Z = -\infty$ to Z_0 represents the acceptance energy (W_a) for the system and must be positive for a nanotube to accept a fullerene by suction force alone. If W_a is negative, then the magnitude of W_a represents the initial kinetic energy needed by fullerene in the form of the inbound initial velocity for it to be accepted into the nanotube. In Fig. 3, we show the acceptance energy W_a for a fullerene and a nanotube of radii in the range 6.1 < a < 6.5 Å. From the figure, W_a = 0 when a = 6.338 Å and nanotubes which are smaller than this will not accept C_{60} fullerenes by suction force alone. This implies that a (10, 10) nanotube (a = 6.784 Å) will accept a C_{60} fullerene from rest, however a (9, 9) nanotube (a = 6.106 Å) will not. The result of this model is well in agreement with Hodak and Girifalco [11] and Okada, Saito and Oshiyama [12].

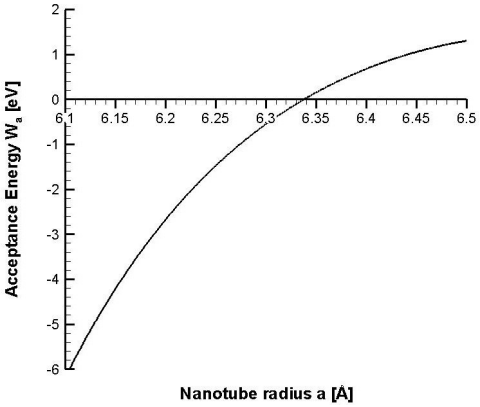

Figure 3. Acceptance energy threshold for a C_{60} molecule to be sucked into a carbon nanotube

The suction energy W for a fullerene, which is the total work performed by the van der Waals interactions on a C_{60} molecule entering a carbon nanotube, can be determined similar to W_a but the integral is performed over the entire range, from $Z = -\infty$ to ∞. In Fig. 4, we plot W for a C_{60} molecule entering a nanotube with radii in the range 6 < a < 10 Å. We note that W is positive when a > 6.27 Å and has a maximum value of W = 3.242 eV at $a = a_{max}$ = 6.783 Å. Accordingly, a (10, 10) carbon nanotube with a = 6.784 Å is

almost exactly the optimal size to maximize W and therefore have a C_{60} fullerene accelerate to a maximum velocity upon entering the tube. Our model predicts that C_{60} molecule in a (10, 10) carbon nanotube will accelerate to a velocity of 932 m/s; this result is in a reasonable agreement with a molecular dynamical simulation of Qian et al. [7], which predict the velocity of 840 m/s for C_{60} molecule entering the tube.

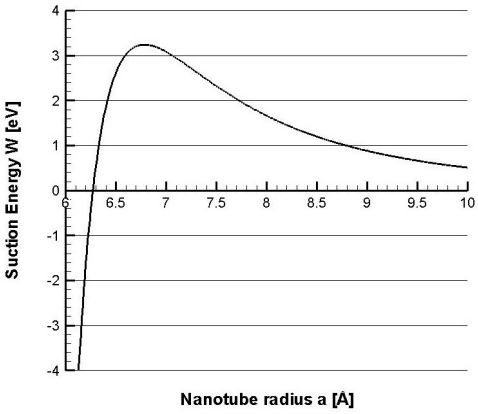

Figure 4. Suction energy for a C_{60} molecule entering a carbon nanotube

IV. Preferred Position of a C_{60} Molecule inside a Single-walled Carbon Nanotube

The preferred position of a C_{60} molecule inside a single-walled carbon nanotube is where the molecule admits the minimum potential energy. Here, we determine this location with reference to the cross-section of a carbon nanotube. In axially symmetric cylindrical polar coordinates, we assume that the fullerene C_{60} of radius b is located at (ε, 0, 0) as shown in Fig. 5, and in a carbon nanotube of infinite extent with a parametric equation ($a\cos\theta$, $a\sin\theta$, z). We note that ε is the distance between the centre of the offset C_{60} molecule and the central axis of the tube, a is the tube radius, $-\pi \le \theta \le \pi$ and $-\infty < z < \infty$.

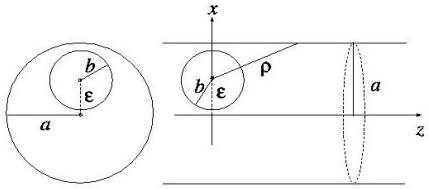

Figure 5. An offset C_{60} molecule inside a carbon nanotube

From Fig. 5, $\rho = (a^2 + \varepsilon^2 - 2a\varepsilon\cos\theta + z^2)^{1/2}$, thus by performing surface integral of (3) over the entire carbon nanotube, we obtain the potential energy E for the offset C_{60} molecule inside the carbon nanotube, namely

$$E = 4\pi^2 ab^2 n_f n_g \left[-\frac{A}{8}(3I_2 + 5b^2 I_3) + \frac{B}{5}\left(\frac{105}{128} I_5 + \frac{1155b^2}{64} I_6 + \frac{9009b^4}{128} I_7 + \frac{6435b^6}{64} I_8 + \frac{12155b^8}{256} I_9\right)\right], \quad (6)$$

where the integrals I_n are defined by

$$I_n = \int_{-\pi}^{\pi} (\alpha - \beta\cos\theta)^{-(n+1/2)}\, d\theta, \quad (7)$$

and $\alpha = a^2 + \varepsilon^2 - b^2$ and $\beta = 2a\varepsilon$. We note that the integrals I_n can be evaluated in terms of elliptic integrals or in terms of hypergeometric functions (see Cox et al. [9]).

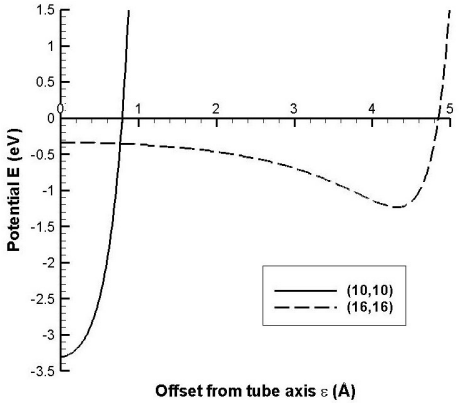

Figure 6. The potential of an offset C_{60} molecule inside a (10, 10) and a (16, 16) carbon nanotubes, with respect to the radial distance ε from the tube axis

In Fig. 6, the potential energy E is plotted with respect to the distance ε. It can be seen that the preferred position for the C_{60} molecule inside a (10, 10) carbon nanotube is where the centre of the C_{60} molecule lies on the tube axis ($\varepsilon = 0$). For a (16, 16) carbon nanotube, we find $\varepsilon = 4.314$ Å. Further, we observe that as the tube radius gets larger, the location where the minimum energy occurs tends to be closer the nanotube wall. These results agree with the findings of Girifalco et al. [10].

V. Oscillation of a C_{60} Molecule inside a Single-walled Carbon Nanotube

In axially symmetric cylindrical polar coordinates (r, z), we assume a C_{60} molecule is located inside a carbon nanotube of length $2L$, centred around the z-axis and of radius a. As shown in Fig. 7, we assume that the centre of the C_{60} molecule lies on the z-axis. This assumption is valid for a (10, 10) carbon nanotube, since the centre of the C_{60} molecule is likely to be on the tube axis due to the minimum potential energy.

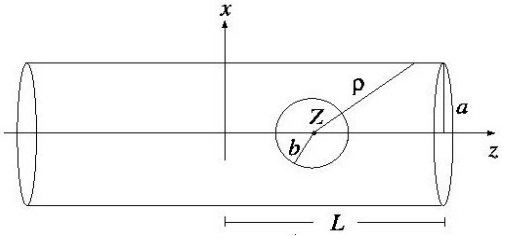

Figure 7. Geometry of the C_{60} molecule oscillation

Here we adopt Newton's second law to describe the oscillatory motion of the molecule inside a single-walled carbon nanotube, namely

$$m_f \frac{d^2 Z}{dt^2} = F_{vdW}(Z), \quad (8)$$

where Z is the distance between the centres of the C_{60} molecule and the carbon nanotube, m_f is the total mass of the fullerene, $F_{vdw}(Z)$ is the van der Waals restoring force, which generates oscillatory motion of the C_{60} molecule. We note that here we neglect the frictional effect, which is reasonable for certain chiralities and diameter of the tube. For example, inside the carbon nanotube (10, 10), the C_{60} molecule tends to move along the axial direction and tends not to suffer the rocking motion due to its preferred location is on the z-axis.

From the symmetry of the problem, we only consider the total axial force in the range $-L \le z \le L$, as such $F_{vdW}(Z)$ in the right hand side of (8) can be replaced by $F_z^{tot}(Z)$,

$$F_z^{tot}(Z) = 2\pi a n_g \left[P(\rho_2) - P(\rho_1)\right], \tag{9}$$

where $P(\rho)$ is defined by (3), $\rho_1 = [a^2 + (Z + L)^2]^{1/2}$ and $\rho_2 = [a^2 + (Z - L)^2]^{1/2}$. In Fig. 8, we plot $F_z^{tot}(Z)$ as given in (9) for a (10, 10) carbon nanotube of length $2L$ = 129 Å, and it can be seen that the force is close to zero everywhere except at the tube extremities. The pulse-like force at the tube ends operates to attract the C_{60} molecule back towards the centre of the tube.

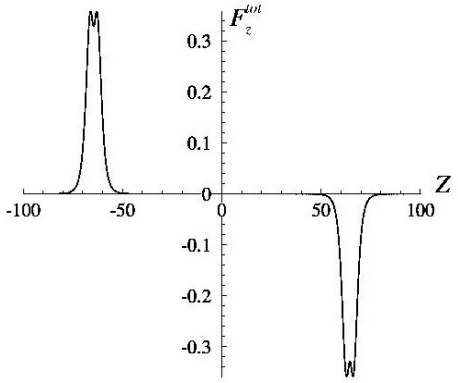

Figure 8. The total axial force for a C_{60} molecule oscillating inside a (10 ,10) carbon nanotube

For $b < a << 2L$, we find that $F_z^{tot}(Z)$ can be estimated by the Dirac delta function. As a result, (8) can be reduced to give

$$m_f \frac{d^2 Z}{dt^2} = W\left[\delta(Z + L) - \delta(Z - L)\right], \tag{10}$$

where W is the suction energy. By utilizing the Heaviside step function, (10) can be integrated to give

$$v = dZ/dt = \left(2W/m_f + v_0^2\right)^{1/2}, \tag{11}$$

for $-L \le Z \le L$, where v_0 is the initial velocity that the C_{60} molecule is fired on the z-axis towards the open end of the tube in the positive z-direction. We note that the initial velocity v_0 is introduced for the case where the C_{60} molecule is not sucked into the tube solely by the suction force due to the strong repulsion. From (11), it implies that the C_{60} fullerene travels inside the carbon nanotube at the constant speed v. As shown in Cox et al. [9], upon using (11) we obtain the velocity v = 932 m/s for the case of the C_{60} molecule initially at rest outside the carbon nanotube (10, 10) and the C_{60} molecule gets sucked into the tube due to the attractive force alone. As such, we obtain the frequency $f = v/(4L)$ = 36.13 GHz. Figure 9 shows the variation of the oscillatory frequency with respect to the nanotube length. This result is in good agreement with the molecular dynamical simulation of Liu et al. [5], which confirms their finding that the shorter the carbon nanotube, the higher the oscillatory frequency.

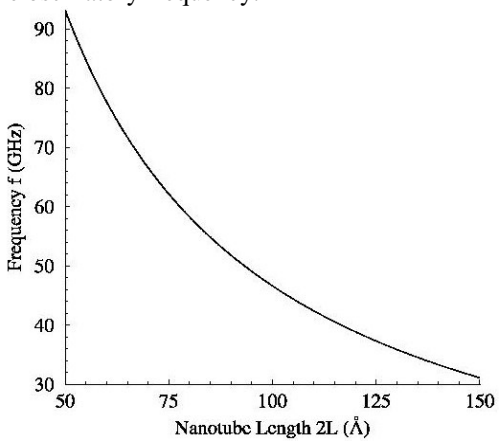

Figure 9. The variation of the oscillatory frequency of a C_{60} molecule with respect to the length of a (10, 10) carbon nanotube

ACKNOWLEDGMENT

The authors are grateful to the Australian Research Council for support through the Discovery Project Scheme.

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